Chaotic wave functions and exponential convergence of low-lying energy eigenvalues

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Abstract

We suggest that low-lying eigenvalues of realistic quantum many-body hamiltonians, given, as in the nuclear shell model, by large matrices, can be calculated, instead of the full diagonalization, by the diagonalization of small truncated matrices with the exponential extrapolation of the results. We show numerical data confirming this conjecture. We argue that the exponential convergence in an appropriate basis may be a generic feature of complicated ("chaotic") systems where the wave functions are localized in this basis.

Statistical properties of complex quantum systems have been studied extensively from various viewpoints. The seminal papers by Wigner [1] and Dyson [2] developed the random matrix theory (RMT [3]) where the systems are considered as members of a statistical ensemble, and all hamiltonians of given global symmetry appear with certain probabilities. The canonical Gaussian ensembles [4,5] correspond to systems with very complicated dynamics when, in almost all bases connected by the transformations preserving global symmetry, the components of generic eigenfunctions are uniformly distributed on the unit sphere in multidimensional Hilbert space. On local scale, Gaussian ensembles predict specific correlations and fluctuations of spectral properties which are in agreement with empirical data for atoms, nuclei [6], quantum dots [7] and resonators (microwave [8] and acoustic [9] experiments). These spectral features are considered usually as signatures of quantum chaos [5,10,11].

Recently, the detail studies of highly excited states in realistic atomic [12] and nuclear [13] calculations demonstrated that such many-body systems are close to the RMT limit although they reveal some deviations, partly due to the presence of the mean field [14], coherent components [15] of the residual interaction and its two-body character [4,16]. In complex atoms and nuclei, precise experimental information exists, as a rule, about low-lying states only. Effective residual interactions , such as the Wildenthal-Brown interaction [17] for the *sd*-shell model turned out to be successful well beyond the input used for their original fit. This justifies the use of such interactions for studying generic complicated states in the region of high level density. The whole shell model approach is based on the large-scale diagonalization even if one is interested in the low-lying states only. The dimensions of matrices increase dramatically with the number of valence nucleons which makes the full diagonalization impractical, even after projecting out correct angular momentum and isospin states. This problem is avoided in the Monte Carlo shell model method [18], but, apart from the so-called sign problem [19] which requires the introduction of an extrapolation when working with realistic interactions, this method is better suited for calculating thermal properties or strength functions than spectroscopic characteristics. In order to consider

individual levels, one needs to supplement the Monte Carlo sampling with some variational procedure including an additional "stochastic" diagonalization ([20] or the QMCD approach [21]). An important step towards larger dimensions in the standard shell model is made with the development of the DUPSM code [22].

Here we suggest a simple approach which allows one, for calculating energies of low lying states, to reduce large dimensions of matrices under study by orders of magnitude, while keeping high precision of the results. The approach is based on the statistical properties of complicated many-body states [12,13]. Because of the strong residual interaction and "geometric chaoticity" [13] of the angular momentum coupling, the eigenstates are extremely complex superpositions of independent particle Slater determinants. However, in contrast to the limiting case of the Gaussian orthogonal ensemble (GOE), the stationary wave functions are not fully delocalized in shell model space. Due to inherently self-consistent nature of the residual interaction (even if it is extracted in a semiempirical manner), its strength does not exceed the typical spacings between single-particle levels which are determined by the mean field, i.e. by the same original forces. Together with the fact that the two-body forces cannot couple very distinct configurations, this leads to a band-like structure of the hamiltonian matrices in the shell model basis.

Theory of banded random matrices did not reach the same degree of completeness as that of canonical Gaussian ensembles. Nevertheless, both mathematical [23] and numerical [24] arguments favor the localization of the eigenstates in Hilbert space, similar to the coordinate localization of electronic states in disordered solids. The generic many-body states in complex atoms or nuclei have a typical localization width [13,24,25]. Inversely, the simple shell model configurations are packets of the eigenstates. Their strength function is fragmented over the range of energies characterized by the spreading width Γ which is nearly constant along the spectrum because the coupling matrix elements between the complicated states are small just as it is needed to compensate small level spacings in the region of high level density [26–28]. The qualitative arguments are confirmed by more general theory [15] as well as by detailed numerical calculations for atoms [12] and nuclei [13,29]. The nuclear

case is close to the strong coupling limit [30,31,13] where the typical width can be estimated [29] as $\Gamma \approx 2\bar{\sigma}$ in terms of the energy dispersion of a simple configuration $|k\rangle$,

$$\sigma_k^2 = \langle k|(H - \langle k|H|k\rangle)^2|k\rangle = \sum_{l\neq k} |H_{kl}|^2. \quad (1)$$

Here H_{kl} are the off-diagonal elements of the residual interaction between the basis states so that the calculation of (1) does not require any diagonalization. The dispersions σ_k of different simple states fluctuate weakly [13] and in our estimate of Γ they are substituted by the appropriate mean value $\bar{\sigma}$ which can be found by the methods of statistical spectroscopy [32].

The practical method of truncating large shell model matrices was suggested in [33]. The shell model states are grouped into partitions (sets of states belonging to the same particle configuration). Since the states separated in energy by an interval broader than Γ are not significantly mixed with the studied state, we truncated the matrix retaining only the partitions whose statistical centroids $\bar{E} = \overline{\langle k|H|k\rangle}$ are closer than 3σ. The spin-isospin projection and the elimination of the center-of-mass admixtures can be done within the truncated subspace only. In order to keep the correct shell model structure, the partitions should be included as a whole. As shown in [33], this method allows for the calculation of low-lying energies with sufficient precision in large shell-model spaces. The truncated eigenvectors overlap with the exact ones on the level of better than 90%.

Going beyond the simple truncation, we consider the convergence of level energies to the exact values as a function of the increasing dimension n of the diagonalized matrix. As an example we take the ^{51}Sc nucleus where the pf-shell model dimensions of $1/2^-$ and $3/2^-$ states are 13016 and 24474, respectively. Spectroscopic information on this radioactive isotope is only tentative providing an interesting experimental and theoretical problem. For the calculations, the FPD6 interaction [34] was used. Fig. 1 shows the calculated energies of the two lowest $3/2^-$ states and two lowest $1/2^-$ states for several values of n ranging from $n = 2000$ to the full dimension N. Already the smallest dimensions lead to a good agreement within few As the dimension increases, in all four cases the running eigenvalue

converges very fast and monotonously to the exact result. The convergence is almost pure exponential, $E(n) = E_\infty + A\exp(-\gamma n)$; typically $A \approx 300$keV, $\gamma \approx 6/N$.

The exponential convergence of eigenvalues would be extremely helpful for shell model practitioners. It would make almost redundant the full large scale diagonalization if one is interested in the low-lying states only. Instead, the calculations for several increasing dimensions (still far from the full value and therefore easily tractable) would end in determining the exponential parameters and simple extrapolation to the exact result. At present, the rigorous mathematical theory of convergence is absent, and we limit ourselves by qualitative arguments and plausible conjectures.

The convergence under consecutive truncations is determined by the type of the matrix and by the original unperturbed basis which orders the basis vectors in a certain way. The ordering is done almost uniquely in the spherical shell model where the mean field is fixed and all many-body states are organized in partitions. For the lowest levels, the admixtures of highly excited states outside of the starting truncation correspond to the wings of the strength function. As confirmed by the atomic [12] and nuclear [13,29] studies, the strength function has in average universal shape. This shape evolves from the standard Breit-Wigner function [35] for the "weak damping" case to the Gaussian form at strong damping (semicircle in the RMT limit of the uniform spectra [15,23] which is not reached in practical cases). Correspondingly, the dependence of the spreading width on the strength of the residual interaction changes from quadratic in the standard golden rule [35] to linear [31,15,29]. The remote wings of the strength function have their own energy behavior [12,29]. With high accuracy they can be described [29] by an exponential function of energy. This is a clear manifestation of the localization of the eigenfunctions typical for the banded hamiltonian structures [36,23]. In this limiting regime, the average local strength is simply proportional to the total remaining strength, $F(E) \approx \mathrm{const}\,[1 - \int^E dE'\, F(E')]$ which gives $F(E) \sim \exp(-\mathrm{const}E)$. The exponentially weak mixing should lead to the exponentially small energy shifts and to the corresponding convergence of the eigenvalues.

We can expect the exponential behavior to be generic for the large matrices of quasi-

banded form with the off-diagonal elements of approximately the same order of magnitude along the spectrum, This conjecture can be checked by generating random matrices with the desired properties and diagonalizing them in a sequence of progressing truncations (the matrices are first ordered according to their diagonal elements). Since there is no "vertical" structure in such random matrices, we do not have here physical arguments concerning the optimal truncation sequence. We show in Fig. 2, left, a typical result for the banded GOE matrix with the width $b = 0.293N$ which clearly demonstrates the exponential convergence. The full GOE matrix, Fig. 2, right, converges more slowly in the absolute sense and does not saturate. This is a simple consequence of the fact that the ground state of a GOE matrix is repelled by the higher states to the edge of the semicircle (-2 with the GOE definition accepted here and in [13]). This process is driven by the off-diagonal elements; all of them in average have the same order of magnitude. Their number and, whence, the dispersion σ, eq. (1), is greater in the full GOE. Therefore the distance from the unperturbed position is also greater in this case (the diagonal and off-diagonal contributions add in quadratures). In all studied cases with the width b changing from $0.1N$ to the full GOE, the convergence is exponential and the exponent γ is approximately scaled inversely proportional to b.

In realistic cases there is also a leading sequence of regular diagonal elements. A similar banded matrix example, considered in [12], goes back to Wigner [1]. The matrix consists of the equidistant diagonal with the spacing D and random off-diagonal matrix elements V_{kl} within the band $|k - l| \leq b$. At relatively weak interaction, $g \equiv \langle V^2 \rangle / D^2 < 1$, the main contribution in the perturbation series for the admixture $w_n = C_n^2$ of a very remote state $|n\rangle$, $n \gg 1$, to the wave function of a low-lying state $|0\rangle$ is given by the summation of long "straight" paths in Hilbert space connecting the initial state with the final one through various intermediate stops. Because of the random character of the off-diagonal interaction, the mean value of w_n is determined by the squares of the contributions of these paths (no interference). In the approximation of a weakly changing level density, this can be approximately written as an integral equation of the random-walk type,

$$w_n = \frac{g}{n^2} f_n + \frac{g}{n^2} \sum_k f_{n-k} w_k \tag{2}$$

where the factor $1/n^2$ comes from the energy denominators, and f_n shows the behavior of typical squared off-diagonal matrix elements V_{n0}^2 as a function of the distance n from the diagonal. With the sharp band boundary [12], the weights w_n decrease very fast, essentially as $\exp(-n \ln n) \sim (n!)^{-1}$. With the smooth cut-off, the convergence is getting closer to exponential. Thus, for the exponential cut-off of the matrix elements, $V_{kl} \sim \exp(-|k-l|/b)$, we have $f_n = \exp(-2n/b)$, and eq. (2) allows a simple solution $w_n = A \exp(-2n/b)/n^2$. Therefore the contributions to energy of the state $|0\rangle$ should converge $\sim nDw_n = DA \exp(-2n/b)/n$. Fig. 3 illustrates this consideration by an example of the numerical diagonalization of a random matrix with the equidistant diagonal and the exponential cut-off. One may note that the rate of convergence is similar to that in the shell model calculation, see above, where the effective width of the band is close to $b \approx N/4$ [13]. However, the method of eq. (2) becomes invalid in the case of strong interaction when the contributions to the perturbation series of additional loops in Hilbert space cannot be neglected. The range of convergence is seen from the expression for the constant in the above solution, $A = g/[1 - g \sum_{k=1} k^{-2}]$, which determines the critical value $g_c = 6/\pi^2$.

It is interesting to test the character of the convergence in simple solvable models. A harmonic oscillator, shifted from the equilibrium position by a constant force, $H = a^\dagger a + \lambda(a + a^\dagger)$, lowers its energy by λ^2. The exact ground state is a coherent combination of unperturbed states $|n\rangle$. In accordance with the composition of the coherent state, the convergence of the energies in the unperturbed basis of the original oscillator is $\sim \lambda^{2n}/n!$. This is clearly seen in Fig. 4, left. The fast convergence is due to the constant level density along the main diagonal while the perturbation has matrix elements growing only $\sim n^{1/2}$. In the case of a quartic anharmonic oscillator, the exponential convergence is modulated with oscillations.

Another example displays the case of the slow convergence. The tight-binding model of a finite one-dimensional lattice has degenerate levels in each of N identical wells and

the amplitude v of hopping between the adjacent wells. The eigenstates of the model are delocalized standing Bloch waves with energies within the band, $E_q = 2v\cos\varphi_q$, $\varphi_q = \pi q/(N+1)$, $q = 1, 2, \ldots, N$. As it is easy to see, the truncation in the site basis corresponds to the convergence $\sim 1/n^2$, see Fig. 4, right.

Tridiagonal matrices with the entries $H_{nn} \equiv \epsilon_n$ and $H_{n-1,n} = H_{n,n-1} \equiv V_n$ smoothly depending on n can be analyzed in a general way using the recurrence relation for the secular determinants $D_n(E)$ of the matrix $(H - E)$ truncated at the nth step,

$$D_n(E) = (\epsilon_n - E)D_{n-1}(E) - V_n^2 D_{n-2}(E). \tag{3}$$

The consecutive approximations $E^{(n-1)}$ and $E^{(n)}$, $n \gg 1$, to a low-lying eigenvalue E are the roots of $D_{n-1}(E^{(n-1)}) = 0$ and $D_n(E^{(n)}) = 0$, respectively. For $\epsilon_n \gg E^{(n)}$ (with a slight modification, the method works also for initially degenerate matrices with ϵ_n =const), the asymptotic behavior of the energy increments $\Delta_n = E^{(n)} - E^{(n-1)}$ follows from (3) as

$$\frac{\Delta_n \Delta_{n-2}}{(\Delta_n + \Delta_{n-1})(\Delta_{n-1} + \Delta_{n-2})} = \frac{V_n^2}{\epsilon_n \epsilon_{n-1}} \equiv \lambda_n. \tag{4}$$

The exponential convergence corresponds to $\lambda_n \to \lambda = \text{const} \neq 0$ at large n (similar increase of diagonal and off-diagonal elements). Then the increment ratio $\xi_n = \Delta_n/\Delta_{n-1}$ also goes to a constant limit $\xi = (1/2\lambda)[1 - (1 - 4\lambda^2)^{1/2}]$ which restricts the exponential convergence region to $\lambda^2 < 1/4$. The existence of the constant limit is still compatible with an additional preexponential factor weakly dependent on n; at large n corresponding fits are usually indistinguishable. An explicitly solvable (by the Bogoliubov transformation) model of the harmonic oscillator with the perturbation $\lambda(a^2 + a^{\dagger 2})$ agrees completely with this estimate. The case $\lambda^2 = 1/4$ corresponds here to the degeneracy of the oscillator with zero frequency, and at $\lambda^2 > 1/4$ the spectrum is inverted. In general, $\lambda = 1/4$ resembles a critical point; the convergence here is described by a power law being exponential outside of this region.

The main difference of the tight-binding case from the oscillator model is the degeneracy of the unperturbed levels (absence of the leading diagonal) which results in the delocalized wave functions of eigenstates. Because of the degeneracy, the analog of eq. (4) contains,

instead of λ_n^2, the ratio $v^2/E^{(n)}E^{(n-1)}$ which is just equal to the critical value $1/4$ in the limit of large n. The situation is similar for the spin chains with the nearest neighbor interaction where the finite size effects on the ground state energy were repeatedly studied [37] and corrections also go as n^{-2}. We expect the presence of disorder (random positions of the original site levels), which leads to the localization of the eigenfunctions, to be accompanied by the transition to the exponential convergence of the eigenvalues.

In conclusion, we discussed the convergence of the low-lying eigenvalues of large matrices describing the realistic many-body hamiltonians of shell-model type. We gave arguments in favor of the conjecture that the exact diagonalization of relatively small matrices, truncated on the grounds of physical partitions and generic spreading widths of simple configurations, provides a starting approximation which can be extrapolated to the exact result with the aid of a simple exponential continuation. The arguments are based on the generic features of quantum chaotic many-body dynamics, simple models and the results of numerical analysis.

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FIGURE CAPTIONS

Figure 1. Energy deviations from the exact shell model result for the lowest excited states $1/2^-$ and $3/2^-$ in ^{51}Sc (diamonds) calculated as a function of the progressive matrix truncation n. Solid lines give a fit $A\exp(-\gamma n)$ with the parameter values $A = 0.26, 0.19, 0.23, 0.35$ MeV and $\gamma = 49.7\times10^{-5}, 47\times10^{-5}, 25\times10^{-5}, 30\times10^{-5}$ for $1/2^-_1, 1/2^-_2, 3/2^-_1$, and $3/2^-_2$, respectively.

Figure 2. Energy deviations for the ground state of random matrices of dimension 1000 as a function of the progressive matrix truncation n (diamonds): the GOE-like banded matrix of the width $b = 0.293N$, chosen in such a way that a half of the matrix elements vanish, approximately in the same proportion as in typical shell model cases, left panel; the full GOE matrix, right panel. Solid lines show a fit $A\exp(-\gamma n)$ with $A = 1.18$ and $\gamma = 3.8\times10^{-3}$, left, and $A = 1.96$, $\gamma = 1.53\times10^{-3}$, right. Note the absence of the horizontal asymptotics in the case of the full matrix.

Figure 3. Convergence of the ground state energy for the banded random matrix with the exponential cut-off of matrix elements $V_{kl}\sim\exp(-|k-l|/b)$ with $b = 0.293N$ (diamonds); the solid line is given by $\mathrm{const}\exp(-2n/b)/n$ which corresponds to the solution of eq. (2).

Figure 4. Convergence of the ground state energy in the tight-binding model of a finite one-dimensional lattice with λ as a hopping parameter, left panels, and for a shifted harmonic oscillator with the hamiltonian $H = a^\dagger a+\lambda(a+a^\dagger)$, right panels. The upper parts show the energy deviation $\Delta E_n = E_0(n) - E_0(\infty)$ as a function of the truncated dimension n (solid lines for $\lambda = 1$ and $\lambda = 2$); dotted lines show the predicted analytical convergence of the models, $\lambda\pi^2/n^2$ (left) and $\lambda^{2n}/n!$ (right). The lower parts characterize the convergence rate $\lambda_n\to\lambda$ by plotting $\lambda_n\equiv\Delta E_n n^2/\pi^2$, left, and $\lambda_n = (\Delta E_n n!)^{1/2n}$, right.

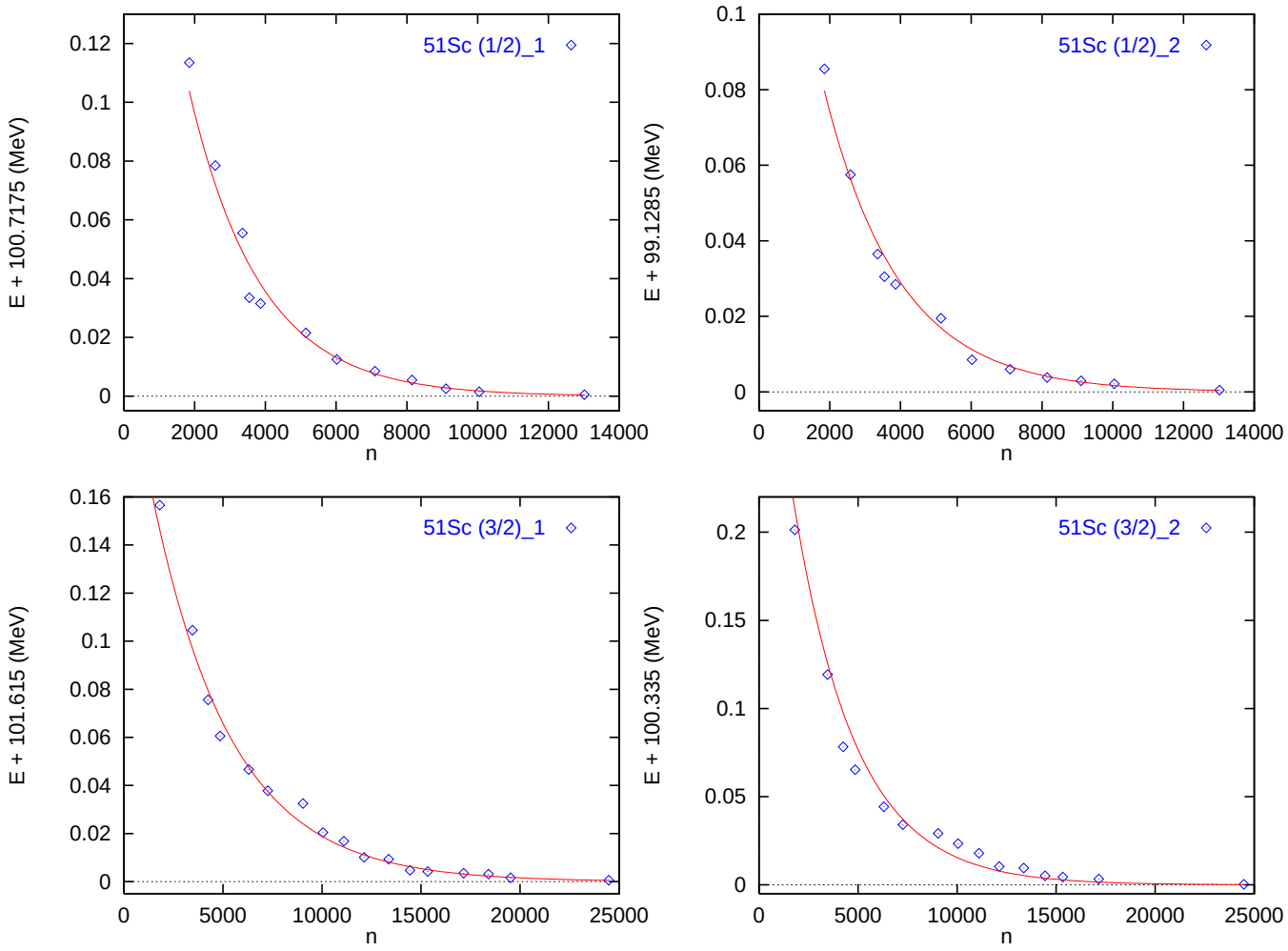
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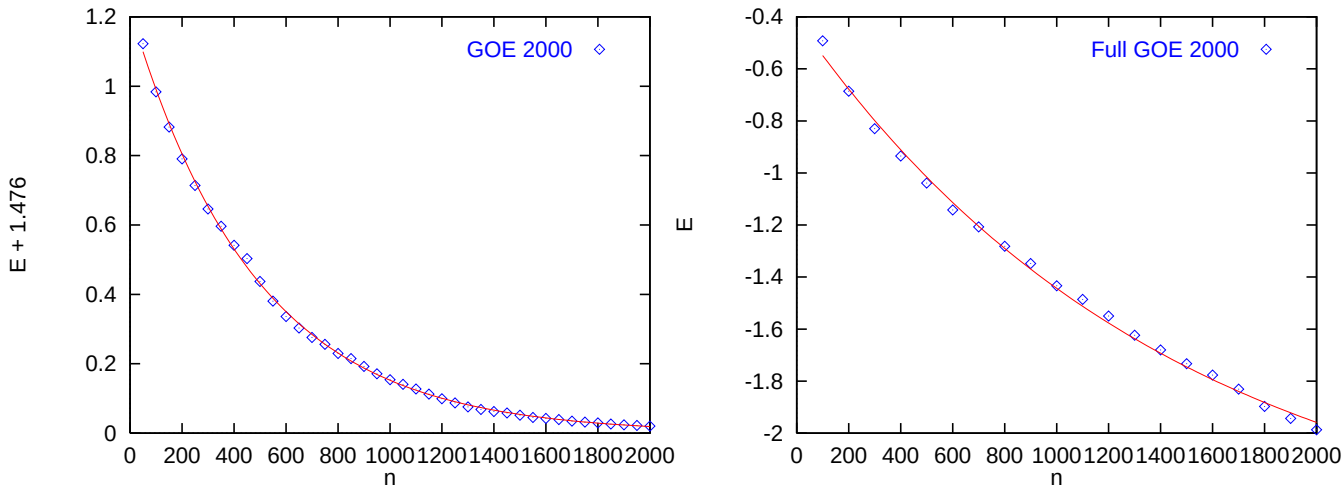
Figure 1:



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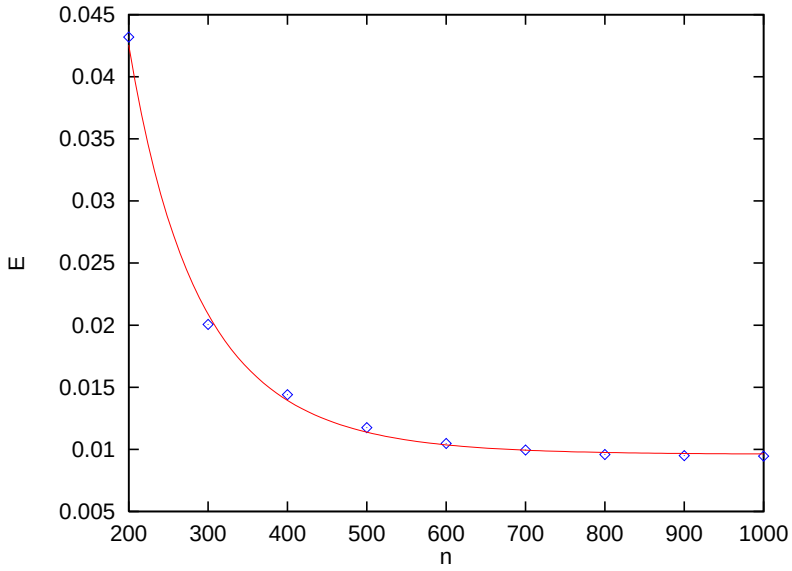
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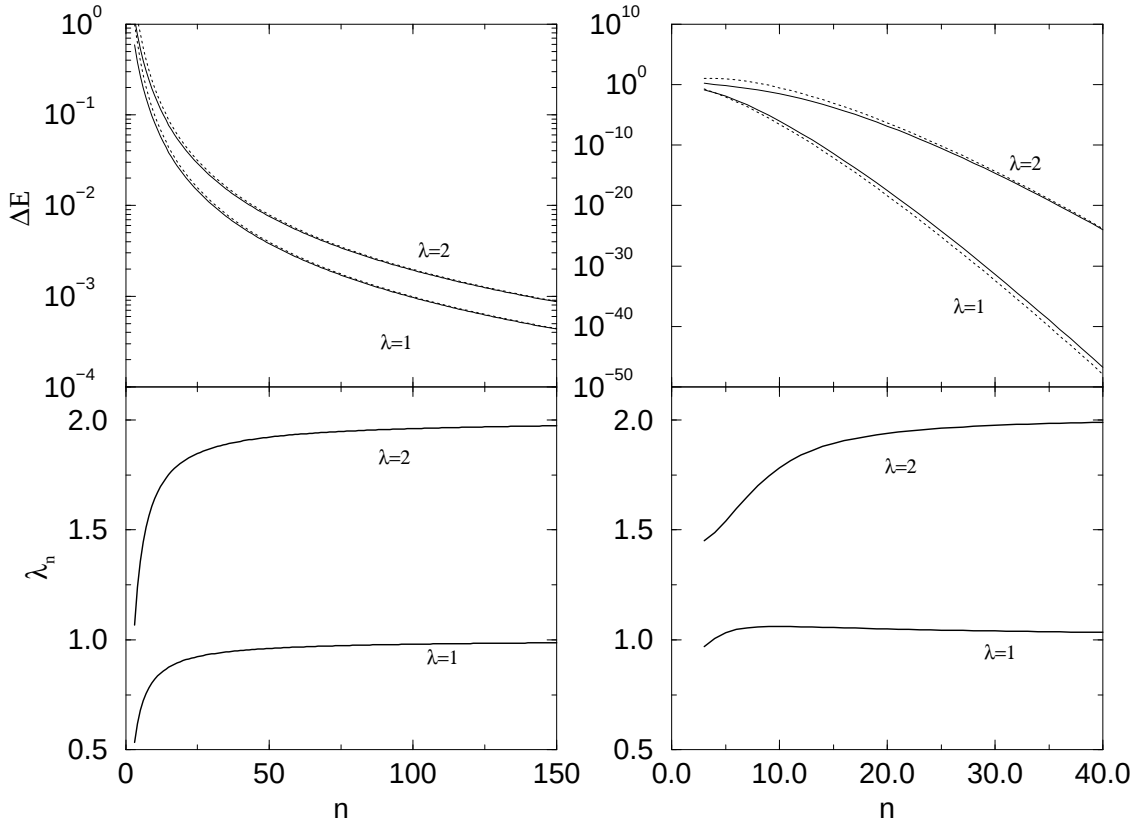
Figure 3: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